There are 2 GOLD runs to the lab

1st Run – 1,000 compounds

2nd Run – 100 compounds

This will be their first time using the GOLD GUI – i.e. the Hermes interface. So, it is their first time with Xming as well.

**TROUBLESHOOTING:**

**We are cheating a little on the ligand set up. We won’t actually minimize these because that would take forever for all of them to do in Maestro or ICM. So, we’ll just use the 3-D structure from PubChem that is close.**

The GOLD GUI will be very SLOOOW. So- they can come back at later times to try again – but they will most likely need a mentor for help.

**IMPORTANT CONCEPTS:**

In drug discovery, we try to find novel compounds that have different structures and properties from drugs that are currently out there (we don’t just want to use the same scaffolds that a bacteria may be resistant to already).

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Finding good positive and negative controls

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